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MODELLING SOIL WATER DYNAMICS IN THE UNSATURATED ZONE: STATE OF THE ART

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ABSTRACT

This paper reviews the principles underlying water dynamics in the unsaturated zone and gives an overview of simulation modelling of soil water flow in the unsaturated zone.

The basic relations describing kinetics of flow and governing equations of flow in the unsaturated zone are presented in a general form considering unsteady multidimensional anisotropic and nonhomogeneous flow in the presence of sinks/sources. The influence of overburden potential, characterizing swelling soils, on water transport through the unsaturated zone is discussed. Outlines of thermally-induced water flow are presented with an extension to the specific case of frozen soils. Complex relationships describing the hydrological system are reduced into the one-dimensional vertical flow cases, for which the mathematical models are defined. The entire model has the form of a set of partial differential equations together with auxiliary conditions, that describe the system's geometry, parameters, boundary conditions and in case of transient flow also the initial conditions. Simulation is defined as operation with such a mathematical model.

Numerical approximations to solve governing equations of unsaturated water flow are emphasized. Recently-introduced numerical methods are discussed pointing out their advantages and limitations. Atmospheric boundary conditions of the modelled system are described with a maximizing procedure of the flux through the soil-air interface. Several options to define lower boundary conditions are discussed and a special type of lower boundary condition is given for the case that unsaturated flow is coupled with a regional groundwater model.

Simulation models require data concerning input, calibration and verification. The current status of collecting model parameters is discussed as well as measurement of common verification data, i.e. phreatic surface, matric head, water content and actual evapotranspiration.

Preferential flow of water through unsaturated soil has considerable consequences for simulating the field water balance. The attempts to simulate such

hydrological systems are also evaluated.

Some transient flow problems are affected by hysteresis. Successful attempts to build hysteresis into dynamic simulation models are still scarce, though recently a number of solutions have been presented.

Finally, several practical examples of simulation of flow problems are presented. These examples are taken from everyday water management practice and document the wide range of applicability of simulation models.

I. INTRODUCTION

Since BUCKINGHAM (1907) introduced the energy concept to describe the condition of water and RICHARDS (1931) formulated the partial differential equation for water flow in unsaturated soil, a quantitative analysis came within reach. Soil water flow, however, is highly non-linear, as both the hydraulic conductivity and the soil water pressure head depend on the soil water content. Exact analytical solutions are only possible for simplified flow cases under a number of restrictive assumptions. Numerical solution of the flow equation on the other hand offers a powerful tool in approximating the real nature of the unsaturated zone for a wide variety of soil systems and external conditions.

The partial differential flow equation can be interpreted numerically by a finite difference, a finite element or a boundary element technique. Then a discretization scheme is applied for a system of nodal points that is superimposed on the soil depth - time region under consideration (Figs. 3 and 4). Implementing the appropriate initial and boundary conditions then leads to a set of (linear) algebraic equations that can be solved by different methods. The operation by means of such a mathematical model is termed simulation, while the model is called simulation model.

The output of a simulation model can include such variables as pressure head, moisture content and flux as a function of soil depth and time. However, most frequently one calculates the terms of the water balance, i.e. infiltration, actual evaporation, actual transpiration, change in soil water storage and the net flux through the region boundary.

The main purpose of using dynamic simulation models is to assess the effects of water management measures such as irrigation, sub-irrigation, drainage, soil improvement and regional water supply plans, on the terms of the water balance of agricultural as well as nature conservation areas. Through the water balance terms one is generally able to evaluate effects of water management on e.g. crop yield and agricultural income. Another application can be found in civil engineering where seepage through dams and seepage losses from channels must be estimated.

Transport of solutes is another aspect, which is directly related to the simulation of unsaturated water flow, i.e. the evaluation of pollution of the groundwater reservoir, salinization, etc.

The yield of a crop well supplied with nutrients is directly related to its water use i.e. to its transpiration. The higher the water use, the higher the yield. Hence simulation of different irrigation regimes by a soil water balance model that has been combined with a crop growth model enables one to find the optimum regime. In such a case the crop and soil system should interact with each other, i.e. crop development with time should have a feedback with calculated actual water use and production rates.

In many soils water shortage for crops is caused by a too shallow rooting depth. The reasons for a restricted rooting depth can be many, such as poor aeration, soil compaction, etc. Again through soil water balance/crop growth models the effects of changes in a soil profile on crop water use and yield can be evaluated.

Inadequate drainage generally results in decreased trafficability and workability of the soil and hence timely farming operations are not possible. The length of the growing season is shortened and consequently crop yield is reduced. If the relationship of soil moisture conditions with farming operations and crop growth is known, one is then able with soil/crop simulation models to evaluate effects of drainage on crop production on a day to day basis. Such an approach is not only feasible for drainage studies, but also for irrigation, soil improvement, etc. and thus applicable to quantitative land evaluation studies in general.

The classical Richards-flow theory upon which most simulation models are based holds for stable flow conditions only. Yet instability of flow has been observed under a wide variety of circumstances such as abrupt and gradual increases of hydraulic conductivity with depth, compression of air ahead of the wetting front and water repellency of the solid phase (e.g. RAATS, 1973). Another example of non-Richards-type of flow is the preferential flow through non-capillary macropores. With classical flow theories one mat then underestimate the velocity and depth of water/solute transport.

The present paper does not review all literature dealing with water flow in unsaturated soil. For example, a subject as transport of solutes is left out of consideration. The main purpose is (i) to give the principles behind unsaturated soil water flow, (ii) to present an outline of simulation approaches and (iii) to consider recent developments. Some examples of simulation of flow problems taken from everyday water management practices are presented.

THEORY OF WATER DYNAMICS IN THE UNSATURATED ZONE

The fact that water moves through an unsaturated soil was recognized by BUCKINGHAM (1907) who related the flow rate to suction gradients. Buckingham also introduced a pressure head term which was later measured by GARDNER and WIDTSOE (1921). RICHARDS (1931) presented the differential equation for soil water flow using an analogy to heat flow in porous media. Up to now this equation is used as the basic mathematical expression that underlies unsaturated flow phenomena.

Mechanical and energy concept

In the mechanical concept only suction gradients were considered as the cause of water movement through the soil. However, water may also move through unsaturated soil by other driving forces such as thermal, electrical, or solute concentration gradients. Therefore, an energy concept has been developed which states that soil water moves in the direction of decreasing energy status.

For a given temperature the energy status of soil water can be characterized by Gibbs' free enthalpy commonly called the water potential. Physically the potential expresses the capacity of a certain mass of water to do work as compared with the same mass of pure free water (defined as having a potential of zero). The soil water potential ϕ can be written as:

$$\phi = \phi_m + \phi_{ex} + \phi_{en} + \phi_{os} \qquad (1)$$

where: ϕ_m = matric potential arising from local interactions between the soil matrix and water

ϕ_{ex} = potential arising from the external gas pressure

ϕ_{en} = overburden (envelope) potential caused by an external load which is partially carried by the soil water phase

ϕ_{os} = osmotic potential arising from the presence of solutes in the soil water

When the water is located at an elevation different from that of the reference level, the gravitational potential ϕ_g has to be added. Hence the total water potential ϕ_t is given by:

$$\phi_t = \phi + \phi_g \tag{2}$$

Potentials can be expressed on a mass, volume, or weight basis. In hydrological studies, the use of potential on weight basis is preferred. The potential then has the dimension of length and is referred to as a 'head' h.

The energy or thermodynamic concept was reviewed by e.g. SLATYER (1967) and TAYLOR (1968). The influence of electrical gradients upon water flow will be incidentally touched on in this review while the dynamics of coupled water and heat flow in unsaturated soils will be given in a separate section.

Kinetics of flow: Darcy's law

Considering multi-dimensional flow under anisotropic and non-uniform conditions, Darcy's law can be written as:

$$\vec{v_i} = -K_{ij}\nabla\phi \quad \text{with } j \text{ (summation index)} = 1,2,3 \text{ for each value of } i \tag{3}$$

where: $\vec{v_i}$ = the flux vector

K_{ij} = the hydraulic conductivity written as a tensor of second degree for anisotropic soil

$\nabla\phi$ = gradient of soil water potential, having a vectorial nature, the soil water potential itself being a scalar

Expressing potential in terms of head, h, and if the only changes in the system are due to interactions between the soil matrix and water, as well as due to elevation x_3, eq. (2) reduces to:

$$h_t = h_m + x_3 \tag{4}$$

For isotropic conditions the Darcy's law (eq. 3) then takes the form:

$$\vec{v}_i = -K \frac{\partial}{\partial x_i} (h_m + x_3) \tag{5}$$

For one-dimensional vertical flow one gets:

$$\vec{v} = -K \left(\frac{\partial h_m}{\partial z} + 1\right) \tag{6}$$

where the notation z for the vertical coordinate (positive upward) is used instead of x_3.

Darcy's law is taking a more complex form when in addition to the water potential gradient another gradient like the electrical or the thermal one is considered. Taking into account the electrical potential gradient, according to the Onsager's phenomenological equations one can write for the coupled one-dimensional water flux v and electrical flux I:

$$v = -L_{11} \frac{\partial h_t}{\partial x} - L_{12} \frac{\partial U}{\partial x}$$

$$I = -L_{21} \frac{\partial h_t}{\partial x} - L_{22} \frac{\partial U}{\partial x} \qquad (7)$$

where U is the electrical potential and L_{ij} are the so-called cross conductivity coefficients (BRAESTER et al. 1971). A similar way of coupling can be applied to the thermal potential gradients and soil water potential gradients. The question of combination of all the acting forces to one term, which is the derivative of some general potential, was investigated by ZASLAVSKY and RAVINA (1968). The dependency of cross conductivity coefficients on forces themselves as well as on the degree of saturation pose the main difficulty of such an approach.

Conservation of mass

Having defined the flux vector $\vec{v}$, the expression for conservation of mass can be written as:

Xurs

$$\text{div } \vec{v} = - \frac{\partial \theta}{\partial t} - S \qquad (8)$$

where θ = the volumetric soil moisture content

t = time

S = the sink (or negative source) of soil water (e.g. water extraction by roots)

For one-dimensional vertical flow eq. (8) reads as:

$$\frac{\partial v}{\partial z} = - \frac{\partial \theta}{\partial t} - S \qquad (9)$$

Differential equation of unsaturated flow

Combination of mass conservation and Darcy's equation leads to the partial differential equation of unsaturated flow. There are a number of alternative expressions of the partial differential equation considering steady and unsteady flow conditions.

Combination of eq. (8) and (3) yields:

Deurs

$$\mathrm{div}\,(K_{ij}\nabla\phi) = \frac{\partial\theta}{\partial t} + S \qquad (10)$$

or

$$\frac{\partial}{\partial x_i}\left(K_{ij}\frac{\partial\phi}{\partial x_j}\right) = \frac{\partial\theta}{\partial t} + S \qquad (11)$$

Eq. (11) describes unsteady multi-dimensional anisotropic and non-homogeneous flow. It should be mentioned that K_{ij} is not only a parameter for an anisotropic and heterogeneous medium, but it also depends on the soil moisture content θ. Substituting eq. (4) into eq. (11) and getting back to isotropic soils, eq. (11) then reduces to:

$$\frac{\partial}{\partial x_i}\left(K(\theta)\frac{\partial h_m}{\partial x_i}\right) + \frac{\partial K(\theta)}{\partial x_3} = \frac{\partial\theta}{\partial t} + S \qquad (12)$$

In eqs. (11) and (12), repeated indexes mean summation on these indexes.

Considering the one-dimensional case of vertical flow and introducing the differential soil water capacity $C(h_m) = \partial\theta/\partial h_m$, eq. (12) can be rewritten in terms of soil matric head h_m as:

$$\frac{1}{C(h_m)}\frac{\partial}{\partial z}\left[K(h_m)\left(\frac{\partial h_m}{\partial z} + 1\right)\right] - \frac{S}{C(h_m)} = \frac{\partial h_m}{\partial t} \qquad (13)$$

Eq. (13) has the advantage of being applicable for the entire flow region, including saturated and partially saturated flow. The use of h_m instead of θ as the dependent variable has the advantage of being applicable in layered soils, where h_m remains continuous at the boundaries between the layers.

Swelling soils

The overburden or envelope potential, as mentioned in eq. (1), plays a role in soils where an applied load is not fully carried by the solid soil particles. In swelling clay soils, the overburden potential resulting from the load of overlying soil layers can be calculated according to GROENEVELT and BOLT (1972) as:

$$\phi_{en} = \int_{P=0}^{P=P} \left(\frac{\partial e}{\partial \vartheta}\right)_{P,T} dP \tag{14}$$

or

$$\phi_{en} = \alpha P \tag{15}$$

where: P = load

$\partial e/\partial \vartheta$ = slope of the shrinkage characteristic

T = temperature

e = void ratio = volume of voids/volume of solids

ϑ = moisture ratio = $(1+e)\theta$ = volume of water/volume of solids

α = load factor

θ = volumetric water content = volume of water/total volume

Both Darcy's equation and the continuity equation remain valid in swelling soils. However, the composition of total potential differs from that in rigid soils and the space coordinate system changes due to swelling and shrinkage. This problem is overcome by defining a material coordinate m according to eq. (16) (PHILIP and SMILES, 1969):

$$\frac{dm}{dz} = \frac{1}{1+e} \tag{16}$$

where: m = material coordinate

The conservation of mass (eq. 9) can then be converted into:

$$\left(\frac{\partial v}{\partial m}\right)_t = -\left(\frac{\partial \vartheta}{\partial t}\right)_m - S \tag{17}$$

Evidently, the mentioned processes not only influence the calculation of water transport through the unsaturated zone, but also the equations governing infiltration at the soil surface (GIRALDEZ and SPOSITO, 1984).

Thermally induced soil water flow

The thermal regime of the soil can affect soil water movement. Several researchers attempted to describe the interaction of thermal and water potential gradients (e.g. HADLEY and EISENSTADT, 1955). MEEUWIG (1964) reported that the dependence of soil water viscosity on the temperature is as much as 3 times higher than of the free water viscosity. Also the soil water diffusivity increases considerably when the soil temperature rises (JACKSON, 1963).

Two different approaches evolved in analyzing the coupling between soil water and heat flow. The mechanistic approach (KRISCHER and ROHNALTER, 1940; PHILIP and DE VRIES, 1957) employs the concepts of fluid mechanics and heat conduction leading, for one dimensional water and heat flow, to:

$$\frac{\partial \theta}{\partial t} = \nabla(D_T.\nabla T) + \nabla(D_\theta.\nabla\theta) - \frac{\partial K}{\partial z} \qquad (18)$$

$$C_s \frac{\partial T}{\partial t} = \nabla(\lambda.\nabla T) - L_v\nabla(D_{\theta_v}.\nabla\theta) \qquad (19)$$

where: D_T = thermal diffusivity

D_θ, D_{θ_v} = total isothermal diffusivity resp. isothermal vapour diffusivity

C_s = volumetric heat capacity

L_v = latent heat of vaporization

λ = thermal conductivity of soil

∇T = temperature gradient

The thermodynamic approach involves the use of thermodynamics of irreversible processes together with the Clapeyron equations to derive the coupling coefficients (TAYLOR and CARY, 1964). BOLT and GROENEVELT (1972) and KAY and GROENEVELT (1974) give a derivation of the basic partial differential equations for the case, when matric potential is considered as a superficial driving force. They indicate that the temperature gradient ∇T could introduce a liquid flow in the opposite direction as compared with the solution by means of the mechanistic approach for the same value of matric head.

TEN BERGE (1986) shows that the widely accepted PHILIP and DE VRIES (1957) formulation of thermally induced liquid flow does not describe the real coupling in the true thermodynamic sense. He gives an outline for combining the mechanistic and thermodynamic approaches to solve coupled soil water and heat flow for bare soil surface conditions.

In arid and semi-arid regions with rapidly drying soils, the application of simultaneous soil water and heat flow principles is essential. An extensive review of coupled water and heat flow in drying soils was presented by WIEGAND and TAYLOR (1961) and BRUTSAERT (1981). Discrepancies between the assumptions used in most theoretical investigations and the prevailing physical conditions in arid areas were reviewed by JURY et al. (1981). A major problem in dealing with water flow in drying soils is the separation between vapour and liquid flow. MENENTI (1984) has shown that thermal convection of soil air can occur in the top layer. Heat and vapour flow can be in opposite direction due to the density gradient induced by vapour production. He related thermal admittance of the soil surface to the thermal properties of the underlying soil layers and considered the soil heat flux as a driving force for upward soil vapour flow under the conditions that evaporation takes place below the soil surface.

Few investigations were reported on thermal effects in liquid dominant processes such as infiltration in irrigated fields. Recently an extensive derivation of the basic equation of coupled water and heat flow in (trickle) irrigated fields was given by GHALI (1986). Although based on the mechanistic approach of PHILIP and DE VRIES (1957) and DE VRIES (1958), Ghali's conceptual model is general and considers radial two-dimensional or one-dimensional systems with hysteresis and both water and heat sinks/sources.

Frozen soils

Frozen soils play a significant role in the hydrology of many watersheds. Pore blockage by ice greatly decreases the permeability of soil and causes large runoff rates from otherwise mild rainfall or snowmelt events. Extreme erosion rates result when such runoff occurs from thawed saturated surface layers overlying a still frozen soil layer. The complex processes characterizing simultaneous heat and soil water transport in a freezing soil were studied by e.g. TAYLOR and LUTHIN (1978), GUYMON et al. (1980), HROMADKA et al. (1981).

The physics of a frozen heterogeneous soil profile includes terms of soil energy balance and soil water balance. Considering conductive, convective and latent heat transfer, the one dimensional energy conservation equation for potentially freezing soil can be written as:

$$\frac{\partial}{\partial z}\left(\lambda(\theta)\frac{\partial T}{\partial z}\right) + \rho_l c_l \frac{\partial (v_l T)}{\partial z} + S_h = C_S \frac{\partial T}{\partial t} - \rho_i L_f \frac{\partial \theta_i}{\partial t} + L_v\left(\frac{\partial \rho_v}{\partial t} + \frac{\partial v_v}{\partial z}\right) \qquad (20)$$

The mass conservation equation reads:

$$\frac{\partial}{\partial z}\left[K(\theta)\left(\frac{\partial h_m}{\partial z} + 1\right)\right] + \frac{\partial v_v}{\rho_l \partial z} + S_m = \frac{\partial \theta}{\partial t} + \frac{\rho_i \partial \theta_i}{\rho_l \partial t} \qquad (21)$$

where: ρ_l = density of liquid water

c_l = specific heat capacity of water

v_l = downward liquid water flux

C_s = volumetric heat capacity of soil

ρ_i = density of ice

L_f = latent heat of fusion

θ_i = volumetric ice content

ρ_v = vapour density in soil pore space

v_v = downward water vapour flux through soil

S_m = water sink/source

S_h = heat sink/source

A complex analysis of the freezing soil-residue-snowpack system is presented by FLERCHINGER and SAXTON (1987). They studied the impact of tillage, residue, solutes and environmental conditions on freezing soil and developed a detailed physically-based model of the system.

A new method based on the total energy concept to solve the problem of combined heat and water flow in partly unsaturated and seasonally frozen soils was given by KARVONEN (1988). He simplified equations (20) and (21) by neglecting the vapour flux terms and derived from the soil water retention curve both a freezing characteristic curve and the relationship between soil temperature and soil water potential in the frozen soil. He proposed both iterative and explicit techniques to calculate unknown unfrozen and frozen water content and soil temperature.

Water extraction by roots

Since GRADMAN (1928) and VAN DEN HONERT (1948) suggested that under steady-state conditions water flow through the soil-root-stem-leaves pathway could be described by an analogue of Ohm's law, the following expression has been widely accepted:

$$T = \frac{h_m - h_r}{R_s} = \frac{h_r - h_l}{R_p} \tag{22}$$

where: T = transpiration rate

h_m, h_r, h_l = matric heads in the soil, at the root surface and in the leaves respectively

R_s, R_p = liquid flow resistances in soil and plant respectively

By considering the diffusion of water towards a single root, GARDNER (1960) showed that R_s is dependent on root geometry, rooting length and the hydraulic conductivity of the soil. This so-called microscopic type of approach is often used when evaluating the influence of complex soil-root geometries on water/nutrient uptake (e.g. DE WILLIGEN and VAN NOORDWIJK, 1987; ZELLER, 1987).

In the field, however, steady-state conditions hardly exist. Moreover, the living root system is dynamic (dying roots are constantly replaced by new ones), geometry is time dependent, water permeability varies with position along the root and with time. Root water uptake is most effective in young root material, but the length of young roots is not directly related to total root length. In addition, experimental evaluation of root properties is hardly practical, and often impossible.

Thus, instead of considering water flow to single roots, a more suitable approach might be the macroscopic one, in which a sink term S representing water extraction by a homogeneous and isotropic element of the root system (volume of water per volume of soil per unit of time) is added to the conservation of mass equation (8). FEDDES (1981), MOLZ (1981) and CAMPBELL (1985) gave an overview of possible S-functions for non-uniform matric potentials. DIRKSEN (1985, 1987) investigated S-functions considering the influence of both the osmotic and the matric potential.

As it seems to be impossible and unpractical to look for a complete physical description of water extraction by roots, FEDDES et al. (1978) described S semi-empirically by:

$$S(h_m) = \alpha(h_m)\, S_{max} \qquad (23)$$

where $\alpha(h_m)$ is a dimensionless prescribed function of pressure head and S_{max} is the maximal possible water extraction by roots. The last mentioned authors assume in the interest of practicality a homogeneous root distribution over the soil profile and define S_{max} according to (see Fig. 1):

$$S_{max} = \frac{T_p}{|z_r|} \qquad (24)$$

where T_p is the potential transpiration rate and $|z_r|$ is the depth of the root zone.

PRASAD (1988) and HAYHOE and DE JONG (1988) take care of the fact that in a moist soil the roots can principally extract water from the upper soil layers, leaving the deeper layers relatively untouched. The root water uptake at the bottom of the root zone (z_r) equals zero and the following solution is derived:

$$S_{max}(z) = \frac{2T_p}{|z_r|} \{1 - \frac{|z|}{|z_r|}\} \tag{25}$$

So far we considered root water uptake under optimal soil water conditions, S_{max}. Under non-optimal conditions, i.e. either too dry or too wet S_{max} is reduced by means of the pressure head-dependent α-function (see eq. 23). The shape of this function is shown in Fig. 2. Water uptake below $|h_{m1}|$ (oxygen deficiency) and above $|h_{m4}|$ (wilting point) is set equal to zero. Between $|h_{m2}|$ and $|h_{m3}|$ (reduction point) water uptake is maximal. Between $|h_{m1}|$ and $|h_{m2}|$ a linear variation and between $|h_{m3}|$ and $|h_{m4}|$ a linear (Fig. 2) or hyperbolic variation is assumed. The value of $|h_{m3}|$ is dependent on the demand of the atmosphere and thus varies with T_p.

MODELLING WATER DYNAMICS IN THE UNSATURATED ZONE

Analogue simulation models

According to PRICKETT (1975) a hydrological simulation model is defined as 'each system that can duplicate the response of a hydrological system'. Simulation models which resemble the real world most closely are physical models (scale models) like for example sand tanks.

Analogue models are based on the similarity between the relations describing water dynamics and those describing physical phenomena such as electrical flow. Examples are the hydraulic and electrical analogues of WIND (1979). Analogue models have the advantage of continuous simulation and they give a good approximation of the exact solution provided that the proper scale factors or transform functions are used. The main disadvantage is the time-consuming construction and operation. At this moment analogue simulation of water flow in the unsaturated zone is rarely applied. However, in combination with digital computers (hybrid models) most of the drawbacks can be overcome.

Mathematical models

In the previous sections the dynamics of soil water was cast in the form of mathematical expressions that describe the hydrological relations within the system. The governing equations define a mathematical model. The entire model has usually the form of a set of partial differential equations, together with auxiliary conditions (REMSON et al., 1971; HORNUNG and MESSING, 1980). The auxiliary conditions must describe the system's geometry, the system parameters, the boundary conditions and, in case of transient flow, also the initial conditions. Operations with such a mathematical model are called simulation.

If the governing equations and auxiliary conditions are simple an exact analytical solution may be found. Otherwise, a numerical approximation is applicable. The numerical simulation models are by far the most applied ones.

Solution of the governing equations

Analytical approach

The relationships that govern the flow of water in unsaturated soil are quasi-linear equations of the parabolic type. Since the coefficients in these equations are functions of the independent variables, exact analytical solutions for specific boundary conditions are extremely difficult to obtain.

Analytical methods to solve the non-linear governing equations (see eqs. 12, 13), search for the exact solution in terms of analytical functions. Such an exact solution, if it exists, requires transformation, separation of variables, and usually a series of error functions.

The commonly used Boltzman transformation reduces the partial differential equations to ordinary differential equations. The Laplace transformation results in removing the time variable. The solution of an equation modified in this way yields a dependent variable as a function of the space variables (GARDNER, 1958). The non-linear mass conservation equation can be analytically solved only using various types of relaxation techniques such as linearization, quasi-linearization and transformation to steady state (BRAESTER et al., 1971; PHILIP, 1968a,b; 1970).

The basic equation that describes one-dimensional vertical water movement in isotropic non-swelling soils with no consideration of sinks/sources can be derived from eq. (12) as:

$$\frac{\delta\theta}{\delta t} = \frac{\delta}{\delta z} [K(\theta)(\frac{\delta h_m}{\delta z} + 1)] \qquad (26)$$

By introducing the soil water diffusivity $D(\theta) = K(\theta)/C(\theta)$ eq. (26) can be written as:

$$\frac{\delta\theta}{\delta t} = \frac{\delta}{\delta z} (D(\theta) \frac{\delta\theta}{\delta z}) + \frac{\delta K(\theta)}{\delta z} \qquad (27)$$

The following simplifications can be introduced to find analytical solutions:

- K is an analytical function of θ or h_m;
- hysteresis is neglected;
- the medium is homogeneous and isotropic;
- the flow is considered to be stationary or a succession of steady-state situations (quasi-stationary approach);
- the gravity force is neglected.

The first two assumptions linked with the third one have resulted in a great number of analytical solutions (e.g. GARDNER, 1958; LOMEN and WARRICK, 1978). The gravity force is often neglected in describing the infiltration process in originally dry soil, resulting in analytical solutions as derived by e.g. PHILIP (1957, 1958), PARLANGE (1971) and PARLANGE et al. (1987).

Numerical approach

With the advance of digital computers, emphasis has shifted drastically from the classical approach of analytical solutions to the rapidly developing field of numerical analysis. At present, numerical approximations are possible for complex, compressible, nonhomogeneous and anisotropic flow regions having various boundary configurations.

Numerical methods are based on subdividing the flow region into finite segments bounded and represented by a series of nodal points at which a solution is obtained. This solution depends on the solutions of the surrounding segments and on an appropriate set of auxiliary conditions.

In recent years a number of numerical methods has been introduced. The methods that are most appropriate to the problem of soil water dynamics, will now be discussed below.

Finite difference methods

Finite difference methods (REMSON, 1971), either explicit or implicit, belong to the most frequently used techniques in modelling unsaturated flow conditions. To illustrate the use of finite difference methods, the one-dimensional case of unsaturated flow without sink/sources (eq. 26) will be considered.

Let the entire flow domain be divided into a grid of equal intervals, Δz and the time domain be similarly divided into intervals Δt. The resulting two-dimensional grid is shown in Fig. 3. Referring to this figure eq. (26) can be expressed in finite difference form as:

$$\frac{\theta_i^{j+1} - \theta_i^j}{\Delta t} = \frac{1}{\Delta z} \left[K_{i+\frac{1}{2}}^j \left(\frac{h_{m_{i+1}}^j - h_{m_i}^j}{\Delta z} + 1\right) - K_{i-\frac{1}{2}}^j \left(\frac{h_{m_i}^j - h_{m_{i-1}}^j}{\Delta z} + 1\right)\right] \qquad (28)$$

where: i = index along the space coordinate

j = index along the time abscissa

Eq. (28) represents the so-called forward difference scheme with an explicit linearization of the $K(\theta)$-function.

The forward difference scheme is easy to program but the solution becomes unstable unless Δt is kept sufficiently small.

In the backward difference scheme, the right hand side of eq. (28) is written for the (j+1)th time level which leads to a set of implicit simultaneous nonlinear algebraic equations. Another implicit set of equations can be obtained by the so-called Crank-Nicholson (time centred) finite difference scheme or by the rather commonly used uncentred scheme (BRAESTER et al., 1971). There are a great number of methods to solve an implicit set of algebraic equations, such as linearization, predictor-corrector or iteration methods. For a complete review, see REMSON et al. (1971) and HORNUNG and MESSING (1981).

In dealing with unsaturated flow problems that involve more than one space dimension and a grid with many nodal points, it is often necessary to use a mixed scheme that relies on simultaneous displacements along one space dimension and on successive displacements along the remaining space dimensions. This leads to the method of successive overrelaxation (SOR) (WATTS, 1970; AMERMAN, 1976). In the case of isotropic conditions, faster convergence may be sometimes achieved by using the iterative alternating direction implicit procedure (ADIPIT) of PEACEMAN and RACHFORD (1955) and of VAUCLIN et al. (1975). HORNUNG and MESSING (1980) developed a mixed implicit ADI-predictor-corrector method to solve a two-dimensional unsaturated flow problem under unsteady conditions.

The advantage of the finite difference method is its simplicity and efficiency in treating the time derivatives. On the other hand, the method is rather incapable to deal with complex geometries of flow regions. A slow convergence, a restriction to bi-linear grids and difficulties in treating moving boundary conditions are other serious drawbacks of the method.

Finite element method

With finite element methods (e.g. ZIENKIEWICS and PAREKH, 1970; ZIENKIEWICZ, 1971; NEUMAN, 1973) the domain is divided into a number of rigid elements. The properties of different element types are described e.g. in ZIENKIEWICZ et al. (1966, 1970). In modelling soil water flow problems, triangular elements can be efficiently used to represent difficult geometries and to concentrate coordinate functions in regions where rapid changes are anticipated - such as near soil surface or wetting fronts. The corners of such triangular elements (Fig. 4) are designated as nodal points. These nodes serve the purpose of locating state variables, e.g. matric heads. Each element is characterized by local coordinate functions (NEUMAN et al., 1975). This permits the application of variational or weighted residual principles (WANG and ANDERSON, 1982). Of the latter, Galerkin's method is the most widely used. It leads to an approximate solution at any given time t in the form:

$$h_m(x_i,t) = \sum_{n=1}^{N} h_{m_n}(t).U_j(x_i) \qquad (29)$$

where: x_i = space coordinate of the node n, i = 1,2,3

N = total number of nodes

U_j = shape function, defined for each element

$h_{m_n}(t)$ = value of h_m at the node n

By applying the following steps of the Galerkin scheme (NEUMAN et al., 1975) one gets a set of quasi-linear first-order differential equations:

$$[A]\{h_m\} + [C].\{\frac{dh_m}{dt}\} = \{Q\} + \{B\} + \{D\} \qquad (30)$$

where: [A] = conductance matrix

[C] = capacity matrix

{Q} = boundary conditions vector

{B} = gravity term vector

{D} = sink term vector

The coefficients of eq. (30) can be obtained by applying the Galerkin method individually for each element and adding up the effects of these elements (see e.g. KARVONEN, 1987).

To integrate eq. (30), the time domain is discretized into a sequence of finite intervals and the time derivatives are replaced by finite differences:

$$[A]_{t+\frac{1}{2}} \frac{\{h_m\}_{t+1} + \{h_m\}_t}{2} + [C]_{t+\frac{1}{2}} \frac{\{h_m\}_{t+1} - \{h_m\}_t}{\Delta t} = \{Q\}_{t+\frac{1}{2}} + \{B\}_{t+\frac{1}{2}} + \{D\}_{t+\frac{1}{2}} \tag{31}$$

where $t+\frac{1}{2}$ implies that the coefficients are evaluated at half the time step to prevent unwanted oscillations (NEUMAN, 1973; NEUMAN et al., 1975). Vector $\{h_m\}_{t+1}$ includes the unknown matric heads which should be solved by assuming that the matric heads at time t are known. The resulting set of equations is then solved, e.g. by Gauss elimination. Due to the nonlinear nature of the equations, the results must be improved by an iterative process. The iteration procedure is stopped when a prescribed degree of convergence is achieved.

Finite element methods are capable of solving complex flow geometries, nonlinear and time-dependent boundary conditions, while they possess a high flexibility in following rapid soil water movement. In many cases the rate of convergence of the finite element methods exceed those of finite difference methods. A drawback of the finite element method is the rather time-consuming and laborious preparation of the solution mesh. However, with an automatic mesh generation model this problem could be considerably reduced. Another problem is that checking the finite element solution by simple calculations is not always possible.

Boundary element method

This method (e.g. BREBBIA et al., 1980) known also as Boundary Integral Equations, presents the most recent application of an approximate method to solve soil water flow problems. The integral of the domain of flow is eliminated by a set of basic functions and therefore reduces the problem to a so-called boundary-only problem. The reduction of the order of differentiation results in considerably less computer storage of matrix coefficients. TAIGBENN et al. (1985) used this method to solve a problem characterized by time-dependent governing equations and boundary conditions. High efficiency and ability to solve singular problems on infinite regions are the advantages of the method. On the other hand, the presence of sinks/sources can increase the matrix size considerably. When dealing with an integration of transcendental functions over a domain, one is also losing the advantage of efficiency.

Initial and boundary conditions

Initial conditions must be defined when transient soil water flow is modelled. Usually values of matric head or soil water content at each nodal point within the soil profile are required. However, when these data are not available water contents at field capacity or those in equilibrium with the groundwater table might be considered as the initial ones.

Upper boundary conditions

While the potential evapotranspiration rate from a soil depends only on crop and atmospheric conditions, the actual flux through the soil surface and the plants is limited by the ability of the soil matrix to transport water. Similarly, if the potential rate of infiltration exceeds the infiltration capacity of the soil, part of the water runs off, since the actual flux through the top layer is limited by moisture conditions in the soil.

Consequently, the exact boundary conditions at the soil surface cannot be estimated a priori and solutions must be found by maximizing the absolute flux (HANKS et al., 1969; FEDDES et al., 1978) i.e.:

$$|v(K,h_m)| \leqslant |ET_p| \tag{32}$$

$$h_m^{lim} \leqslant h_m \leqslant 0 \tag{33}$$

where: $v(K,h_m)$ = actual upward flux through the soil-air interface

ET_p = the known potential surface flux (i.e. potential evapotranspiration), time dependent

h_m^{lim} = minimum allowed pressure head at the soil surface, time dependent

Methods to calculate ET_p are published elsewhere (e.g. MONTEITH, 1965; PRIESTLEY and TAYLOR, 1972; FEDDES et al., 1974, 1975) and are beyond the scope of this review.

The value h_m^{lim} can be determined from equilibrium conditions between soil water and atmospheric vapour:

$$h_m^{lim} = \frac{RT}{Mg} \ln(f) \tag{34}$$

where: R = universal gas constant ($J.mol^{-1}.K^{-1}$)

T = absolute temperature (K)

M = molecular weight of water ($kg.mol^{-1}$)

g = acceleration due to gravity ($m.s^{-2}$)

f = relative air humidity (fraction)

The possible effect of ponding has been neglected so far. In case of ponding, usually the height of the ponded water as a function of time is given. However, when the soil surface is at saturation then the problem is to define the depth in the soil profile where the transition from saturation to partial saturation occurs (WOODING, 1968).

There are different ways to partition the potential evapotranspiration, ET_p, into potential transpiration T_p and potential soil evaporation E_p. Usually, one separates E_p from ET_p by taking into account that part of the radiation energy which reaches the soil surface after having passed through the soil cover. For details, see RITCHIE (1972) and BELMANS et al. (1983).

FEDDES (1987) and KABAT et al. (1988) presented the partitioning of ET_p into potential transpiration T_p and potential soil evaporation E_p as a function of leaf area index. The soil water conditions were found to have considerable influence on the partitioning function.

BOESTEN and STROOSNIJDER (1986) developed a simple parametric model to estimate daily actual soil evaporation from the cumulative potential evaporation. The advantage of such a simple model is that the procedure to maximize flux (see eq. 32) is replaced by empirical relations.

When seepage faces are considered, another kind of atmospheric boundary condition should be defined. Along such faces, the pressure is atmospheric and the matric head zero. Since seepage faces vary with time, again an a priori prediction of this phenomenon is impossible and an iterative solution becomes necessary.

In most of the dynamic transient models, the surface nodal point is treated during the first iteration as a prescribed flux boundary and matric head h_m is computed. If h_m satisfies eq. (33), the upper boundary condition remains a flux boundary during the whole iteration. If not, the surface nodal point is treated as a prescribed pressure head in the following iteration. Then in case of infiltration, $h_m = 0$ and in case of evaporation $h_m = h_m^{lim}$. The actual flux is then calculated explicitly and is subject to the condition of eq. (32).

Lower boundary conditions

At the lower boundary one can define three different types of conditions:

a) Dirichlet condition: the pressure head is specified;

b) Neumann condition: the flux is specified;

c) Cauchy condition: the flux is a function of a dependent variable.

The phreatic surface (place, where matric head is atmospheric) is usually taken as lower boundary of the unsaturated zone in the case, where recorded water table fluctuations are known a priori. Then the flux through the bottom of the system can be calculated. In regions with a very deep groundwater table, a Neumann type of boundary condition is used.

Dirichlet condition

Easy recording of changes in phreatic surface in case of present groundwater table is the main advantage of specifying a zero matrix head as the bottom boundary. A drawback is that with shallow groundwater tables (<2 m below soil surface) the simulated effects of changes in phreatic surface are extremely sensitive to variations in the soil hydraulic conductivity.

The nodal points in a soil profile usually have fixed positions and probably none of them will coincide with the water table level. The nodal point, where the matric head is prescribed, is often the one immediately beneath the phreatic level. When large fluxes across the lower boundary occur, an error is introduced by this approximation. The problem of hydrodynamic circumstances which can occur at the bottom boundary was analyzed e.g. by JENSEN (1983).

Neumann condition

A flux as lower boundary condition is usually applied in cases where one can identify a no-flow boundary (e.g. an impermeable layer) or a free drainage case. In the latter case the flux is always directed downward and the gradient $\delta h_t/\delta z = 1$, so the Darcian flux is equal to the hydraulic conductivity at the lower boundary.

Cauchy condition

This type of boundary condition is used when unsaturated flow models are combined with models for regional groundwater flow or when the effects of surface water management are to be simulated. Writing the lower boundary flux, v_b, as function of the phreatic surface, which is in this case the dependent variable, one can incorporate relationships between the flux to/from the drainage system and the height of the phreatic surface. This flux-head relation can be obtained from drainage formulae such as those of HOOGHOUDT (1940) or ERNST (1962) (see SKAGGS, 1980) or from regional groundwater flow models (e.g. VAN BAKEL, 1986).

With the lower boundary conditions the connection with the saturated zone can be established. In this way effects of activities influencing the regional groundwater system upon, for instance, crop transpiration can be simulated. The coupling between the two systems is possible by considering the phreatic surface as an internal moving boundary with one-way or two-way relationships. For a full survey, see VAN BAKEL (1986).

The most general form of the Cauchy condition can be written as:

$$v_b = v_d + v_a \tag{35}$$

where v_b is the flux through the lower boundary, v_d is the flux from/to the drainage system and v_a is the flux to/from deep aquifers (Fig. 5). The flux v_d can be written as a sum of drainage fluxes of different order:

$$v_d = - \sum_{n=1}^{N} \frac{h_{t1,n} - h_{t2}}{\Upsilon_n} \tag{36}$$

where $h_{t1,n}$ is open water level (below the soil surface), h_{t2} is phreatic surface and Υ_n drainage resistance of drainage system of order n (ERNST, 1978).

The seepage flux v_a can be expressed in terms of a resistance flow as:

$$v_a = - \frac{h_{t3} - h_{t4}}{c} \tag{37}$$

where h_{t3} is the level of the phreatic surface averaged over the area, h_{t4} is the piezometric level of the deep aquifer and c is vertical resistance for flow between phreatic and deep aquifer.

When the Cauchy-condition is linked with a one-dimensional vertical flow model, one can consider such a solution as quasi-two-dimensional, since both vertical and horizontal flow are calculated.

COLLECTION OF DATA FOR MODEL INPUT AND VERIFICATION

Required input data

Simulation of water dynamics in the unsaturated zones requires input data concerning the model parameters, the geometry of the system, the boundary conditions and, when simulating transient flow, initial conditions. With geometry parameters the dimensions of the problem domain are defined. With the physical parameters the physical properties of the system under consideration are described. With respect to the unsaturated zone it concerns the soil water characteristic, $\theta(h_m)$, and the hydraulic conductivity, $K(\theta)$. If root water uptake is also modelled, the parameters defining the relation between root water uptake and soil water status should be given, together with crop specifications. In case a functional flux-head relationship is used as lower boundary condition the parameters describing the interaction between surface water and groundwater and - if necessary - the vertical resistance of poorly permeable layers have to be supplied.

Soil physical properties

The most important soil physical properties for water movement in the unsaturated zone are the relationships between the soil matric head (h_m), water content (θ) and hydraulic conductivity (K).

During the last 50 years many methods were developed to determine these relationships in situ and from soil samples in the laboratory (see KLUTE, 1986). Traditionally these methods need a steady-state flow or some equilibrium situation at different matric heads. The procedures are very time consuming and they determine the h_m-θ and the K-h_m relationships on different soil cores. A much faster method was developed by WIND (1966) and BOELS et al. (1978) to determine both the h-θ and the K-θ relationships from a transient flow experiment on one evaporating soil sample.

KOOL et al. (1987) reviewed recent developments in parameter estimation techniques for unsaturated flow. The parameters of an a-priori formulated model, which describes the K-h_m-θ relationships, are estimated from a transient flow experiment with known initial and boundary conditions. The observations of the experiment (e.g. matric heads, outflow) and the model-predicted output are compared. The estimated parameters of the model are optimized to minimize the differences between the observations and predicted output. The advantage of this approach is that no restrictive initial and boundary conditions are needed. Therefore this technique can be also used in field studies. But one should realize that the hydraulic processes are as well described as the K-h_m-θ-model used allows for. Another problem is that the estimated parameters are not necessarily the most optimal ones and that the solution can be dependent on the initial estimates.

Software has been developed to estimate the five parameters of the Van Genuchten model from transient flow experiments (VAN GENUCHTEN, 1980). Extensions can be added to include hysteresis and air entrapment (KOOL and PARKER, 1987). In the latter case the K-h_m-θ relationships are described by eight parameters. The present authors use Wind's type of evaporation experiment and some additional information (e.g. the volumetric water content at saturation and at a matric head of -15 000 cm) to determine the K-h_m-θ relationships by parameter estimation. The estimates are compared with the more direct calculations following Wind's method (Fig. 6). In this way one can estimate the physical characteristics of a soil sample and check whether the postulated model with its estimated parameters can describe the observations sufficiently well.

A new method to estimate the vertical and horizontal hydraulic conductivity based on the inverse approach has been developed by KARVONEN (1988). The method applies a simplification of the Kalman filtering technique (MAYBECK, 1979). The advantages of the simplified Kalman filtering technique are that (i) it allows to assess uncertainty involved in the parameter estimates, (ii) it reveals the dependence of the parameters on state variables and (iii) it allows to test time invariancy of the parameters.

Spatial variability and scaling

Most models for the unsaturated zone are one-dimensional. However, the problems which have to be modelled, are in general of local or regional nature. In that case, we face the problem of spatial variability. This phenomenon recently has attracted much attention in literature (NIELSEN et al., 1973; WEBSTER, 1984, 1985; RUSSO and BRESLER, 1981; JURY et al., 1987a). The basic assumption is that the porous medium is regarded as a macroscopic continuum with properties that are continuous functions of the space coordinates. A set of measured values is interpreted as a realization of a spatial stochastic function. Usually semivariograms are used to specify the spatial structure. The estimation of these functions may be very complicated (JURY et al., 1987a).

Especially with respect to sampling techniques, described by the various authors, the usefulness of the (geo)statistical approach is obvious. But also the application of geo-statistics with regionalization of point simulations is of value. A proper application of the geo-statistical approach may reveal field characteristics that are not apparent from conventional statistical analysis.

A phenomenon connected with regional application of one-dimensional simulation models is scaling. In principle scaling is a technique of expressing the statistical variability in, for instance, the hydraulic conductivity in handsome relationships. By this simplification, the pattern of spatial variability is described by a set of scale factors, defined as the ratio between the characteristic phenomenon at the particular location and the corresponding phenomenon of a reference soil (HOPMANS, 1987a,b). See also JURY et al. (1987b).

Model verification

Verification (or validation) of a model means to check whether or not it is acceptable as an image of reality. This has to be done by comparing observed and simulated variables, such as heights of the phreatic surface, matric head, water contents and actual evapotranspiration. The measurement of these variables will be discussed in some detail.

Height of the phreatic surface

The height of the phreatic surface can be measured by piezometers. By the use of pressure transducers it is easy to record this level automatically. However, water table fluctuations are often recorded with mechanical water table recorders, which may suffer from slow response in rather impermeable soils.

Matric head

In relatively wet conditions ($-800 < h_m < 0$ cm) the matric head can be directly measured by means of a tensiometer connected to a pressure transducer. Below the tensiometer range the matric head can only be measured by indirect methods.

Using electrical resistance blocks (with a range of $-10\ 000 < h_m < -20$ cm), made of gypsum or nylon, one is measuring the electrical resistance of these blocks as an indication of the matric head. The resistance depends on the amount of water in the blocks and the electrical conductivity of the water. The former is dependent on the water retention characteristic of the block and the matric head, which should be in equilibrium with that of the surrounding soil. The conductivity of the water depends on the amount of electrolytes in it. This amount can vary with that of the soil solution. The resistance blocks must be calibrated against soil matric head.

The vapour pressure of soil water can be determined with psychrometers. But this pressure is dependent on both the matric head and the salt concentration of the soil water. The measurement itself is difficult and needs thermal equilibrium between the sensor and surrounding soil. Reasonable results can be obtained only with very low matric heads, i.e. $h_m < -2000$ cm.

Promising developments are based on the thermal conductivity (PHENE et al., 1971; PHENE et al., 1987; range $-3000 < h_m < -100$ cm) and the dielectrical properties (HILHORST, 1986; range $-15{,}000 < h_m < -10$ cm) of a material which is in hydraulic equilibrium with the surrounding soil.

Soil water content

The water content of a soil cannot be directly measured with automatic recording systems. Some property of the soil-water-air mixture is measured which is related to the water content. Consequently, there is always a need for calibration. Relating the water content with the matric head can give serious errors due to hysteresis.

Neither the commonly used neutron probe nor the gamma radiation measurement technique can be used in automatic systems because of safety precautions.

Good results have been obtained with the capacitive method (HILHORST, 1984) which is based on the measurement of capacitance of a capacitor with the soil-water-air mixture as the dielectric medium. The water content can be determined after field calibration with an accuracy of ± 0.02 $m^3.m^{-3}$ (HALBERTSMA et al., 1987). The changes in the water content can be used to calculate daily evapotranspiration as the unknown term of the water balance (Fig. 7).

A similar method that uses the dielectrical properties of the soil is time domain reflectometry (TDR), applied in soil physics by TOPP et al. (1980). The propagation time of a pulse travelling along a wave guide is measured. This time is dependent on the dielectrical properties of the soil surrounding the wave guide and consequently dependent on the water content of the soil. Determination of this time is more difficult than the frequency measurement of the capacitive method. The accuracy of both methods is comparable. Note that the TDR method can be used for many soils without calibration, because the relationship between the apparent dielectric constant and volumetric water content is only weakly dependent of soil type, soil density, soil temperature and salt content (TOPP and DAVIS, 1985a,b,c). TOPP et al. (1980) reported a measured volumetric water content with an accuracy of ± 0.02 $m^3.m^{-3}$.

Because of the ever expanding computer power, numerical simulation models can describe the physical processes with increasing accuracy in time and space. This gives a need in the future for more continuous and accurate data collection. Only automatic recording systems can do this job.

Many data acquisition units are commercially available. These units can be used as front ends of a computer system or as independent units with data logging facilities. With these units the recording of data is not a limiting problem. The limitations are still on the side of the sensors that have to convert the soil water status into electrical signals.

Increasing attention has been paid to the spatial distribution of the measuring sites to obtain statistically representative data sets. Here, a linkage with remotely sensed surface soil water contents seems to point out a future direction (GURNEY and CAMILLO, 1984).

Actual evapotranspiration

There are three potential sites to measure actual evapotranspiration ET - the soil, the plant and the atmosphere. Soil-based measurements, where actual evapotranspiration is estimated indirectly as the rest term of the water balance (eq. 38), have been the most popular.

The change in water storage ΔW for a given period of time Δt can be written as the difference of inflow, i.e. infiltration, net upward flow through the bottom Q, and outflow i.e. evapotranspiration ET:

$$\Delta W = I + Q - ET \qquad (38)$$

The problem with eq. (38) is that it is very difficult to evaluate Q properly. This flow is the resultant of capillary rise and percolation. Often one does not consider capillary rise: what has percolated through the root zone is simply lost. In the presence of a groundwater table that influences the moisture conditions in the root zone, eq. (38) is usually too simple to apply. One then also has to take into account the water transport in the subsoil below the root zone.

Because of uncertainties in estimation of Q the period for which the evapotranspiration term is calculated from eq. (38), should be sufficiently long (HALBERTSMA et al., 1987).

A common technique for measuring ET from water balances is by lysimetry. The precision of the weighing lysimeter provides the current standard against which other ET measuring techniques are judged. However, there are problems inherent in the use of lysimeters. These include the expenses involved in installation, the limited number of sites that can be maintained, the time required to test different crops, and the care which must be taken to maintain lysimeter conditions which are representative of the surrounding field.

Another measurement site is the plant itself. Possible approaches include xylem flow measurement and remote sensing techniques. However, transpiration measurements neglect the soil evaporation component of ET.

Remote sensing can provide an indirect measure of ET. Using thermal infrared images from satelite or airplane observations, surface temperatures are derived and transformed into daily evapotranspiration values using surface energy balance models. NIEUWENHUIS et al. (1985) proposed to replace the surface-air temperature difference by the instantaneous temperature difference near midday between a crop that is transpiring under condition of restricted soil moisture availability and a crop that is transpiring under optimal moisture conditions (T_c-T_c^*). The net radiation term was recalculated as the 24-hour potential evapotranspiration rate of the crop. Using these adjustments one obtains:

$$ET_a/ET_p = 1 - B(T_c-T_c^*) \tag{39}$$

where ET_a and ET_p are respectively the actual and potential 24-hour evapotranspiration rate and B is a calibration constant, which is crop dependent THUNNISSEN, 1984a; NIEUWENHUIS et al., 1985).

The last group of methods is represented by techniques for atmospheric measurement of ET in the plants' microenvironment. These include chamber techniques, the Bowen ratio method, and the eddy correlation method. The chamber approach often requires cumbersome equipment, and the presence of the chamber can significantly disturb the plant environment.

The eddy correlation method (BRUTSAERT, 1982; KIZER and ELLIOTT, 1987) is attractive because it has a sound theoretical foundation and measures the evaporative flux directly. Major obstacles to its use have been the availability, cost and portability of the required instrumentation.

Under certain conditions fluxes from the surface can be measured by correlating the vertical wind fluctuations with fluctuations in the concentration of the transported entities such as heat, water vapour, CO_2, etc. For sensible, H, and latent heat flux, L_e, the covariances of vertical wind velocity, w, air temperature, T, and vapour density, q, are formed

$$\overline{H} = \rho c_p \overline{w'T'} \tag{40}$$

$$\overline{L_e} = \lambda \overline{w'q'} \tag{41}$$

where ρ and c_p are the density and specific heat of air, and λ is the latent heat of vaporization. The overbarred variables are time averages and those with primes are instantaneous deviations about the time averages.

Equations (40) and (41) describe the turbulent flux components and represent surface fluxes only when the mean component is (by definition) zero i.e., $\overline{w'} = 0$. This assumption is invalid downwind from obstacles or large changes in surface roughness. If a one-dimensional sensor is used to measure w, the vertical alignment is critical because fluctuations in the horizontal wind appear as fluctuations in the measured w. The method has potential to be used over dry lands, under wet conditions is still susceptible to errors.

The Bowen Ratio energy balance method (CAMPBELL SCIENTIFIC, INC., 1987; TANNER and GREENE, 1987) is a means of partitioning the energy budget to determine evapotranspiration (ET). The energy budget is based upon the principle of conservation of energy, where energy entering the surface is equal to energy leaving that surface. The energy budget for a soil or water surface is:

$$R_n - G - H - L_e = 0 \tag{42}$$

where R_n is net radiation for the surface, G is the rate of storage of heat in the soil or water, H is the sensible heat flux, and L_e is the latent energy flux due to evaporation. The sign convention used here is R_n positive into the surface and G, H and L_e positive upward from the surface. R_n is measured with a net radiometer and G is measured with heat flux plates, usually in conjunction with temperature measurements, H and L_e depend on eddy or turbulent transport.

The ratio of the sensible to latent heat flux is called the Bowen ratio (β). Substituting for H in equation and solving eq. (42) for L_e yields:

$$L_e = \frac{R_n - G}{1 + \beta} \tag{43}$$

L_e and H are expressed as:

$$L_e = \frac{\rho c_p}{\gamma} \frac{(e_1 - e_2)}{r_v} \tag{44}$$

$$H = \frac{\rho c_p (T_1 - T_2)}{r_H} \qquad (45)$$

where ρc_p is the volumetric heat capacity of air, γ is the psychrometer constant, e_1, e_2, and T_1, T_2 are the vapour pressures and temperatures at heights z_1 and z_2, and r_v and r_H are the vapour and heat transfer resistances between heights z_1 and z_2. The psychrometer constant is equal to $pc_p/(\lambda\epsilon)$; p is barometric pressure, c_p is the heat capacity of air, λ is the latent heat of vaporization, and ϵ is the ratio of the molecular weight of water vapour to the molecular weight of dry air.

Assuming $r_v = r_H$, the Bowen ratio is given by:

$$\beta = \frac{pc_p (T_1 - T_2)}{\gamma\epsilon(e_1 - e_2)} \qquad (46)$$

and is obtained by knowing the atmospheric pressure and by measuring temperature and vapour pressure at two heights. While barometric pressure can be measured at the site, it is unlikely that it will vary by more than a few percent. In practice, it is generally adequate to calculate the barometric pressure for the site elevation, assuming a standard atmosphere, or to obtain a reading from a nearby station and correct it for any difference in elevation between the reporting station and the Bowen ratio site.

When the Bowen ratio approaches -1, the denominator in eq. (43) approaches 0, causing the calculation of L_e and H to 'blow up'. Fortunately, in the field this situation usually occurs only when H is small, e.g. at night when there is little available energy (R_n - G). In practice, when β is close to -1 (e.g., $-1.25 < \beta < -0.75$), L_e and H are assumed to be negligible and are not calculated.

EXTENSION TO PREFERENTIAL FLOW AND HYSTERESIS

Preferential flow

Most simulation models for the unsaturated zone consider the soil to be isotropic and homogeneous. The fact that most soils are neither was recognized already in the 19th century (SCHUMACHER, 1864; LAWES et al., 1882, as quoted by BEVEN and GERMANN, 1982). In field soils, transport of water is often heterogeneous with part of the infiltrating water travelling faster than the average wetting front. This has important consequences for simulating the field water balance and therefore on the calculation of crop water use, yield, solute transport and pollution of groundwater and subsoil. In some soils preferential flow occurs through large pores in an unsaturated soil matrix, a process known as bypass flow or shortcircuiting (HOOGMOED and BOUMA, 1980). In other soils, different flow rates vary more gradually, while matrix and preferential pathways cannot be distinguished easily.

Preferential flow of water through unsaturated soil can be caused by different mechanisms, one of them being the occurrence of non-capillary sized macropores (BOUMA, 1981; BOUMA and DE LAAT, 1981; BEVEN and GERMAN, 1982). This type of macroporosity can be caused by shrinking and cracking of the soil, by plant roots, by soil fauna or by tillage operations. The occurrence of wetting front instability, as caused by air entrapment ahead of the wetting front or by water repellency of the soil (RAATS, 1973; HENDRICKX et al., 1988) can also be viewed as an expression of preferential flow. Whatever the cause of preferential flow, the result is that the basic partial differential equation (eq. 11) describing flow within the soil matrix domain, needs adaptation.

HOOGMOED and BOUMA (1980) developed a model to simulate infiltration, including preferential flow, into clay soils with shrinkage cracks. The model combines vertical and horizontal infiltration. It is physically based but has only been applied to 20 cm soil cores and has not been tested in field soils. VAN AELST et al. (1986) adapted the SWATRE model for use in cracking clays by calculating water flow through cracks, which was dependent on the water content of the topsoil. BRONSWIJK (1988) introduced the shrinkage characteristic in the simulation model FLOWEX (BUITENDIJK, 1984). The model calculates swelling and shrinkage and corresponding cracking and subsidence in relation to changes in water content. In this approach preferential flow through shrinkage cracks is calculated in dependency of both the area of cracks at the soil surface and the maximum infiltration rate of the soil matrix between the cracks. A one-year field experiment yielded good agreement between simulation and field observations of water balance, cracking and subsidence of a heavy clay soil.

The partitioning of soil water over the soil matrix and macropores, and the fate of water flowing downward through the macropores is handled differently by the various models mentioned above. The common principle of all these models, however, is essentially the two-domain concept. This concept was rejected by BEVEN and GERMANN (1984), who applied kinetic wave theory to model water flow through soils with numerous different sized macropores. Their approach predicts in outflow rates of unsaturated soil cores, but does not yield profiles of soil moisture.

An important aspect of prefential flow is the interaction between water in the soil matrix and water inside the macropores. In some models the total preferential flow is accumulated at the bottom of the macropores and is then added to the unsaturated zone at that depth (BRONSWIJK, 1988; PEERBOOM, 1987; VAN AELST et al., 1986). A more general model was suggested by KABAT, PEERBOOM and BRONSWIJK (1988, personal communication) who linked preferential flow and matrix flow by extending eq. (13) to the form:

$$\frac{1}{C(h_m)} \frac{\partial}{\partial z} [K(h_m)(\frac{\partial h_m}{\partial z} + 1)] - \frac{S}{C(h_m)} + \frac{B}{C(h_m)} = \frac{\partial h_m}{\partial t} \qquad (47)$$

where B represents a source of soil water due to horizontal infiltration. or a sink due to evaporation through the walls of the macropores. For the resulting model see Fig. 8. Because this approach is physically based, it seems promising and generally applicable. However, a quantification of the B-term in eq. (47) poses a difficult problem and requires a number of simplifications when the one-dimensional Richards's type of flow model is considered. A quasi-two-dimensional deterministic approach can be followed to obtain an estimate of the B-term.

EDWARDS et al. (1979) proposed a two-dimensional model which allows for vertical infiltration from the soil surface and for lateral infiltration from a vertical hole after excess precipitation on the surface runs into the opening. Further research is needed under field conditions with sequential wetting and drying cycles.

Hysteresis

Most simulation models ignore the effect of hysteresis. However, it has been recognized for a long time that hysteresis in the soil water retention curve influences the soil water movement, especially when frequent changes from wetting to drying occur (MILLY, 1982; HOPMANS and DANE, 1986). The hysteresis phenomenon does not affect the $K(\theta)$-relation very much and it usually neglected. Note that if $K(\theta)$-functions are not taken as subject to hysteresis, they might be considered being dependent on temperature.

The main reasons for hysteresis in the water retention curve are the complexity of the pore-space geometry, the presence of entrapped air, shrinking and swelling and thermal gradients. The first mathematical models of hysteresis were based on the so-called independent domain concept (POULAVASSILIS, 1962; TOPP and MILLER, 1966). The basic assumptions of this concept are (i) a difference in the water volume of each pore does not depend on matric head and (ii) the pore space is built up of pores or domains with each pore size defined by two soil matric heads.

TOPP (1971b) tested the independent domain concept and reported discrepancies when a high soil water content was considered. He solved the problem (see also POULAVASSILIS and CHILDS, 1971) by introducing a domain dependence factor, so that the drying and wetting of single pore was made dependent on the neighbouring pore status. MUALEM (1974) introduced a model to compute hysteresis, based on the independent domain principle. In 1984, he defined a domain dependence factor as the ratio between the volume of pores actually emptied and the volume which could have been emptied if all the pores would receive enough air from neighbouring pores. In Mualem's model, the volumetric water content for any value of matric head can be calculated from the value of matric head at the last reversal point of the curve. The main drying and wetting curve as well as a domain-dependence factor, have to be defined a priori (MUALEM, 1984). Between these main curves, intermediate scanning curves are followed after each change in external conditions. HOPMANS and DANE (1986) incorporated the hysteresis model of Mualem in a soil-water flow model and they investigated the combined effect of hysteresis and temperature on soil-water movement.

Since there are infinitely many scanning curves, the differential soil water capacity (see also eq. 13) cannot be uniquely defined. Here, the differentiation of Mualem's expressions with respect to matric head can be used at any point of a scanning curve. Usually, the calculations of wetting and drying scanning curves are done at a reference temperature, using experimentally derived relations for the conversion to the actual temperature (HOPMANS and DANE, 1985).

A similar analysis as described above was used by GHALI (1986), who considered hysteresis and simultaneous flow of water and heat, allowing multidimensional transient flow to be modelled. Due to the high flexibility of Ghali's model, the influence of hysteresis terms on different transient flow situations can be investigated.

From a modelling point of view the results of HOPMANS and DANE (1986) are interesting since they found the effect of hysteresis on soil water distribution was dependent on the type of upper boundary condition applied. Soil water flow was more affected by hysteresis (and varying temperatures) for a pressure head boundary condition than for a prescribed flux at the soil surface.

Apart from the examples given, successful attempts to build the hysteresis problem into dynamic simulation transient flow models are still scarce. However, some of the practical problems, e.g. low pressure/very frequent irrigation or significant shrinkage/swelling clearly define a range of flow situations, where hysteresis cannot be omitted. For the case when water retention is noticeably affected by heavy swelling/shrinking and water adsorption-desorption, the boundary hysteresis curves do not join even for the highest values of matric heads (SHCHERBAKOV, 1985). Under such condition all of the present hysteresis models still need adaptations.

EXAMPLES OF APPLICATIONS

Example 1: Seepage through an earth dam

NEUMAN et al. (1975) and FEDDES et al. (1975) have developed the model UNSAT2 which solves transient flow in saturated-unsaturated soil by a Galerkin-type finite element approach. The model can handle flow regions delineated by irregular boundaries and composed of non-uniform soils having arbitrary degrees of local anisotropy. Flow can be considered in the vertical plane, in the horizontal plane, or in a three dimensional region with radial symmetry. A multi-dimensional sink term is incorporated to account for water uptake by plant roots. UNSAT2 has been applied to complex field situations in agricultural and civil engineering problems. DAVIS and NEUMAN (1983) used UNSAT2 to calculate infiltration through an earth dam.

The simulated earth dam has a sloping clay core, sandy shells and a drainage blanket. The following assumptions were made:

- no evaporation or infiltration takes place at the dam surface;
- the drainage blanket is free draining;
- the bottom line of the dam forms an impermeable boundary;
- at time zero the water level is instantaneously raised to 4 metres above the bottom line; at t = 184 hours the water table starts to rise at a constant rate, and at t = 374 hours a height of 12 m is reached. This height remains further constant.

Fig. 9a shows a cross section of the dam and the finite element mesh applied. Fig. 9b presents the simulation output, i.e. the advance of water table inside the dam with time. An important aspect of this problem is e.g.

the assessment of the stability of the downstream sloping shell.

Example 2: Field water use and potato crop yield

Transient water flow in a heterogeneous soil - root system which may or may not be under the influence of groundwater can be described by the model SWATRE (FEDDES et al., 1978; BELMANS et al., 1983). Potential and actual growth rate of a potato crop having optimal nutrient supply can be calculated with the model CROPR (FEDDES et al., 1978). FEDDES et al. (1984) have combined both models into one model, SWACRO, which generates a simulation of the actual development of the potato crop.

By means of this model simulations of the water balance and crop yield of potatoes were carried out. For details see KABAT et al. (1988). During 1981 and 1982, a potato crop was grown on a humous top soil overlying coarse sand. During both growing seasons a complete data set was collected consisting of meteorological measurements, soil-physical characteristics, moisture status in the layered soil profile and crop characteristics. The groundwater table was too deep to influence the plant-soil system. In addition sprinkling was applied while allowing different desiccation limits of the soil. Both simulated and measured values of the cumulative evapotranspiration during 1981 are plotted in Fig. 10a. Water storage within the root zone during the same season is presented in Fig. 10b. Finally the transpiration limited potato crop yield (both total dry matter and tuber yield) obtained during the growing season of 1981 is presented in Fig. 10c.

Additionally simulation of different irrigation regimes was carried out to find the optimum regime (Fig. 10d). Simulations were performed for the 1981 and 1982 growing season with the natural precipitation being 209 and 182 mm respectively. The actual transpiration was computed and the application irrigation efficiency (defined as the ratio of the difference in transpiration between irrigated and not-irrigated crop over the amount of water applied) was plotted against the netto total irrigation gift. The obtained water-use efficiency curves, in spite of their dependency on a certain combination of crop, soil and climate, represent unique information for studies about irrigation management (KABAT et al., 1988).

Example 3: Water supply plan

The economic feasibility of expanding the water supply for agriculture in a region in the northeastern part of The Netherlands was investigated (WORKING GROUP 'TUS-10-PLAN', 1988).

A range of water supply plans was evaluated using a model approach that can be summarized as follows:

- the region was divided into 200 different sets of combinations of soil type, hydrological properties and land use;
- each set (see Fig. 11) of the region was modelled with a special version of the SWATRE-model, i.e. extended by a module for open water level manipulation; operational rules for open water level manipulation were derived from a case study;
- with a historical record of weather conditions over 1954-1983 the effect of water supply on subsurface irrigation and sprinkler irrigation upon actual transpiration was calculated for each set;
- the results were converted into effects on crop yield and agricultural benefits (see Fig. 12). On this basis, favourable areas for water supply could be located.

Example 4. Integration of remote sensing with a water balance simulation model

A method for automatic mapping of evapotranspiration from digitally recorded reflection and thermal images has been tested in combination with simulation models. Crop temperatures derived from heat images were transformed into daily evapotranspiration values by using surface energy models (SOER, 1980; NIEUWENHUIS et al., 1985). These values, however, characterize the hydrological conditions only at one day, while hydrologists are more interested in the cumulative effects of human-imposed activities on crop yield. Therefore, the SWATRE-model was used in order to investigate how far the actual evapotranspiration at that particular day is representative for the entire growing season. The daily values of evapotranspiration derived from the heat images were compared with the simulated values at the same day for different locations within the study region. Twelve out of fourteen locations showed good agreement (see Fig. 13). It was concluded that an important improvement of the hydrological description of an area can be achieved by combining simulation results of a model for the unsaturated zone with remote sensing (NIEUWENHUIS, 1986).

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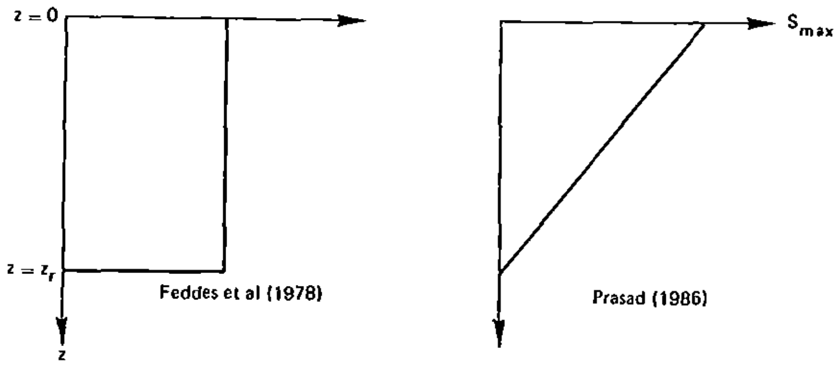

Fig. 1. Schematic view of different water uptake functions under optimal soil moisture conditions, S_{max}, as a function of depth $|z|$, as proposed by FEDDES et al. (1978) and PRASAD (1988). z_r = depth of root zone

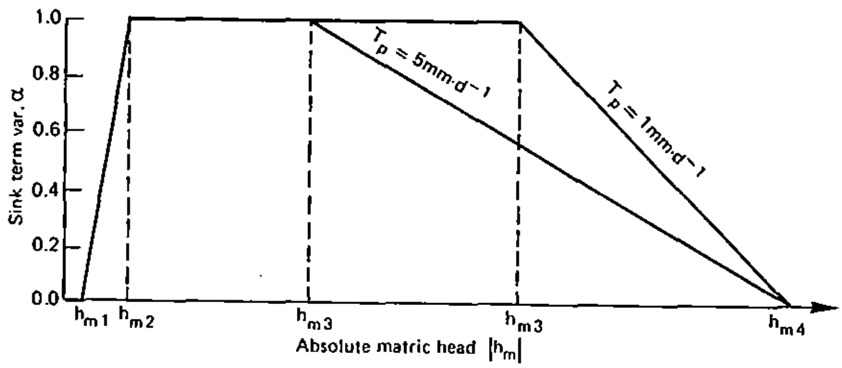

Fig. 2. Dimensionless sink term variable α as a function of the absolute value of the soil water matric head $|h_m|$ (after FEDDES et al., 1978). Water uptake below $|h_{m1}|$ (oxygen deficiency) and above $|h_{m4}|$ (wilting point) is set zero. Between $|h_{m2}|$ and $|h_{m3}|$ (reduction point) water uptake is maximal. The value of $|h_{m3}|$ varies with the potential transpiration rate T_p

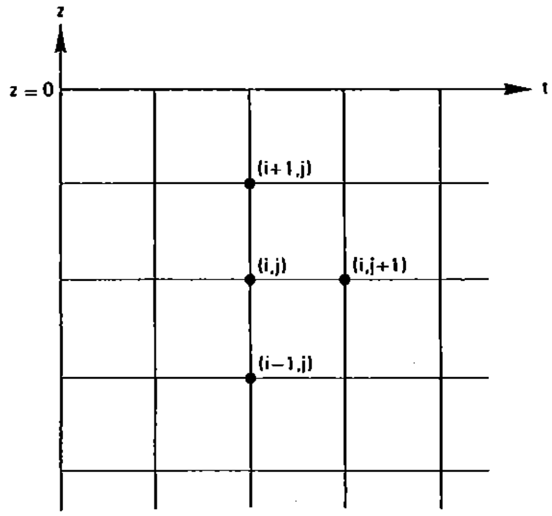

Fig. 3. Bi-linear grid superimposed on the z-t plane with the flow and time domain divided into equal intervals. The grid represents a forward fin~~al~~ite difference scheme

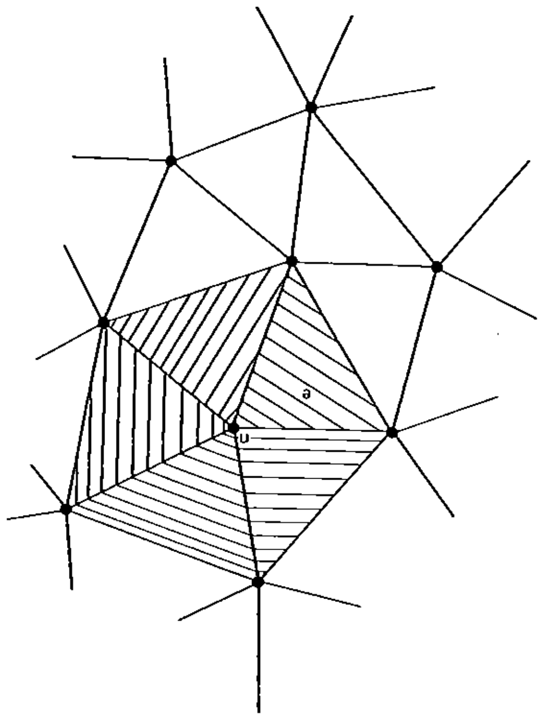

Fig. 4. Network of triangular final elements. The corners of element 'e' are designated as nodal points 'n', in which state variables are located

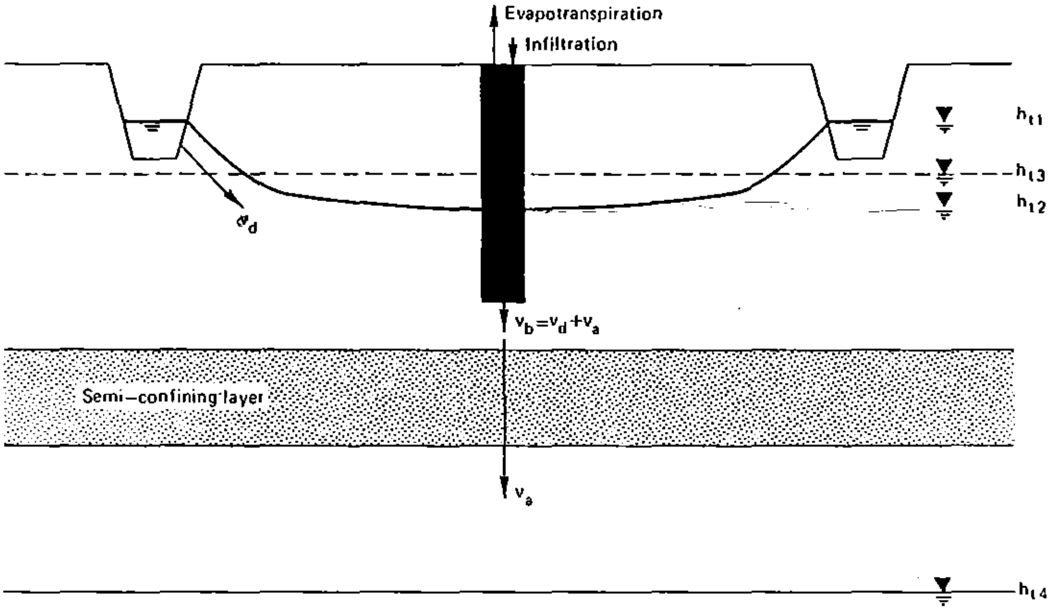

Fig. 5. A representation of the flow situation (Cauchy lower boundary condition, see eq. 35) for the case of outflow from ditches and downward seepage to the deep aquifers; h_{t1} is open water level, h_{t2} is phreatic surface level, h_{t3} is level of the phreatic surface averaged over the area and h_{t4} is piezometric level of the deep aquifer

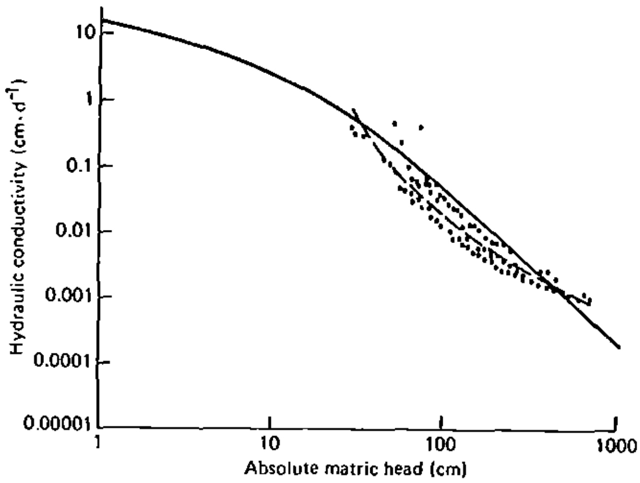

Fig. 6. The hydraulic conductivity K of a soil core as a function of absolute matric head $|h_m|$ determined in the laboratory by Wind's method (WIND, 1966) and by parameter estimation. The dots indicate the calculated conductivities and the broken line describes these points with a second order polynomial. The data of this experiment supplemented with the water contents at matric heads of -2500 and -15 800 cm are used to estimate the parameters of the VAN GENUCHTEN model (1980) with the SFIT program (KOOL and PARKER, 1987). This conductivity is indicated by the continuous curve (parameter estimation from Lafolie and Van Genuchten; personal communication)

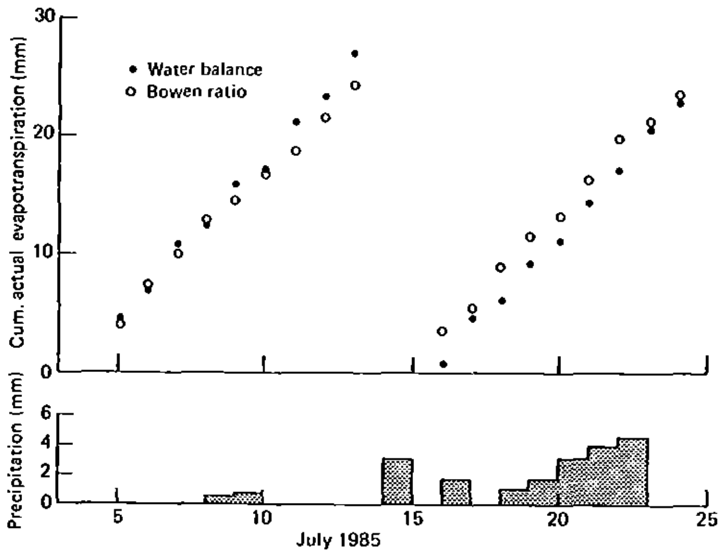

Fig. 7. Cumulative evapotranspiration of maize for two 9-day periods as calculated with a water balance approach and with the Bowen ratio method. The change in water storage of the profile was determined with the capacitive soil water content meter with an accuracy of 0.02 $m^3.m^{-3}$ (after HALBERTSMA et al., 1987)

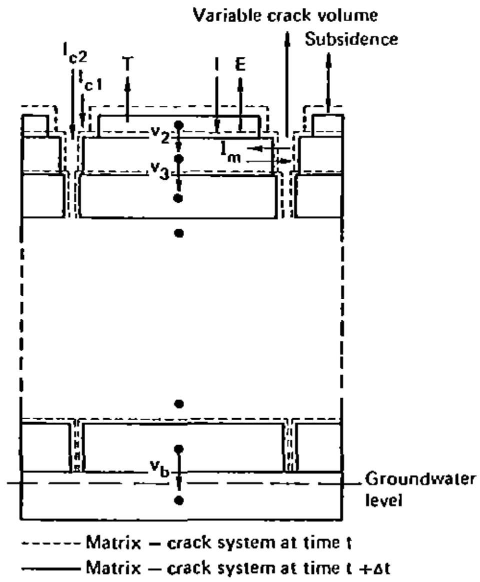

Fig. 8. Schematic presentation of a simulation model for unsaturated water transport in cracking soils. 'I' represents the infiltration rate into soil matrix, $I_{c,1}$ part of total crack infiltration caused by rainfall intensity exceeding the infiltration rate of soil matrix $I_{c,2}$ part of total crack infiltration caused by rainfall directly into the cracks, I_m is horizontal flux through the walls of macropores, E is actual evaporation, T is actual transpiration, v is Darcy flux between two nodal points and v_b is the bottom flux of the system

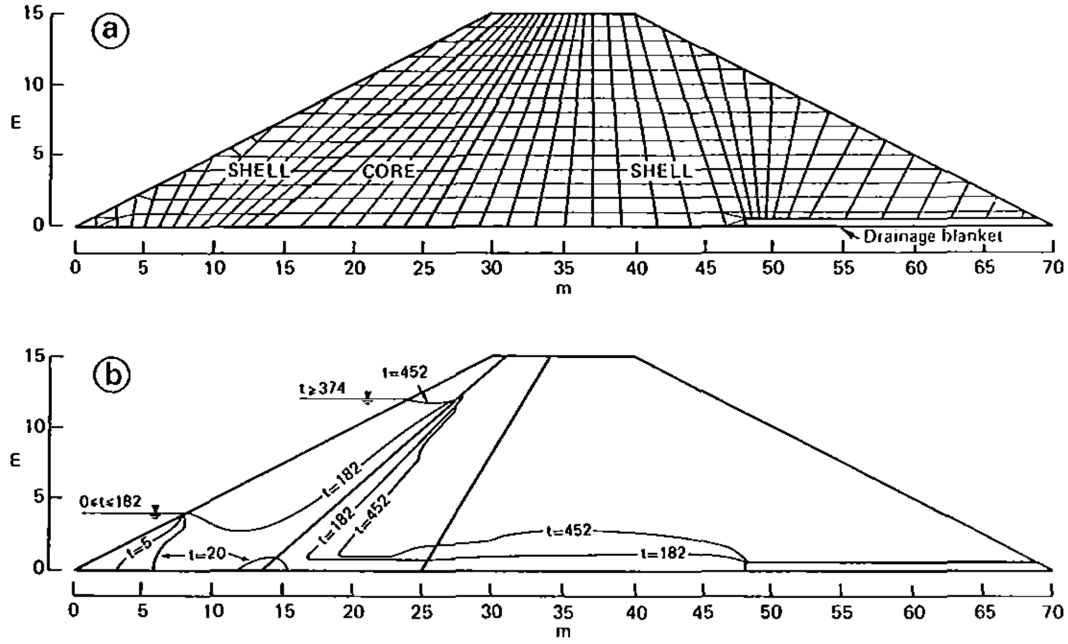

Fig. 9. Seepage through an earth dam as simulated with the model UNSAT2 (after DAVIS and NEUMAN, 1983). Cross section of the dam and the superimposed finite elements grid (a) and advance of phreatic water table inside the dam with time (hours) (b)

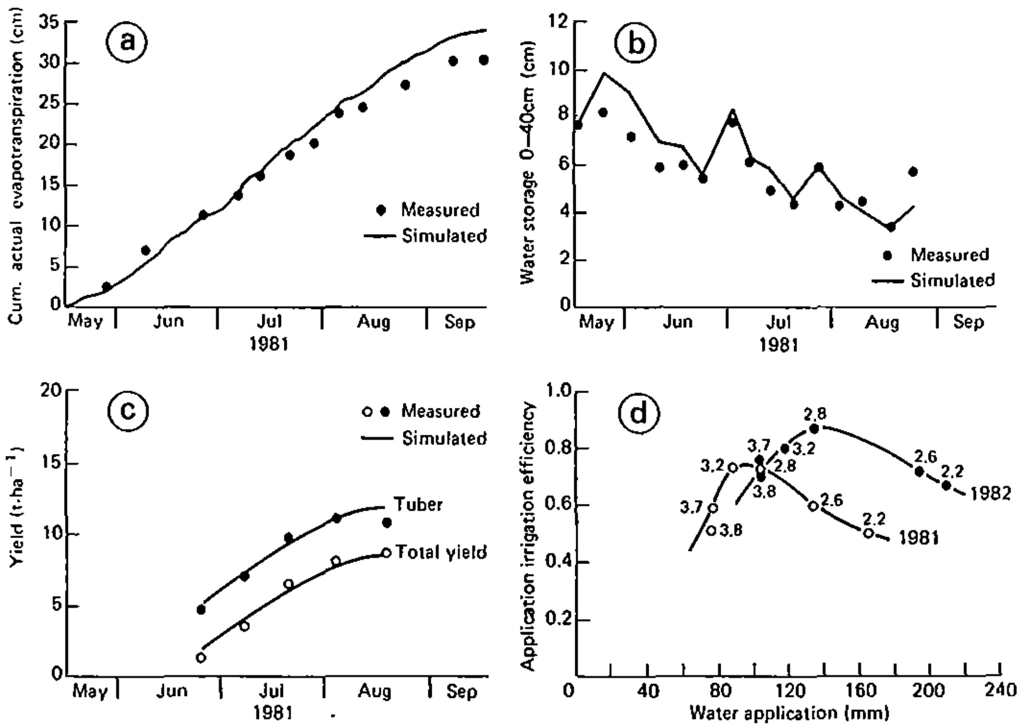

Fig. 10. Field water use and potato crop yield simulated with the model SWACRO (after KABAT et al., 1988). Simulated cumulative actual evapotranspiration (cm) (a) and water storage in the root zone (cm) (b) during the growing season 1981 show good agreement with the in-situ measured values. Calculated and measured dry matter potato yield are presented in (c). Different irrigation regimes were simulated for desiccation limits indicated along the lines (expressed in pF = $\log|h_m|$ and the optimum regime was defined (d)

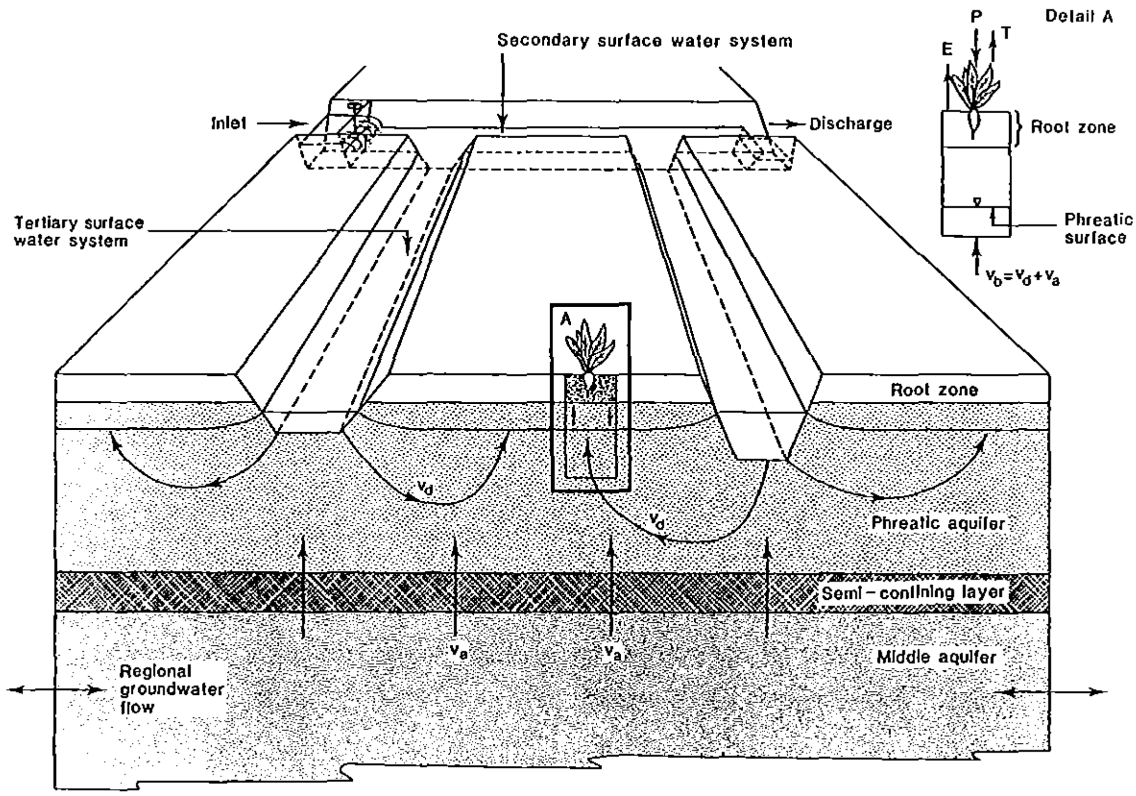

Fig. 11. Schematic representation of the modelled hydrological system as used in the water supply plan (after VAN BAKEL, 1986). Effects of surface water level manipulation on groundwater and crop transpiration were simulated. The upper boundary conditions are defined by transpiration (T) and soil evaporation (E). These are calculated with standard meteorological data, soil physical data and information about crop. The lower boundary condition (Cauchy condition, see eq. 35) is the volume flux density through this boundary v_b

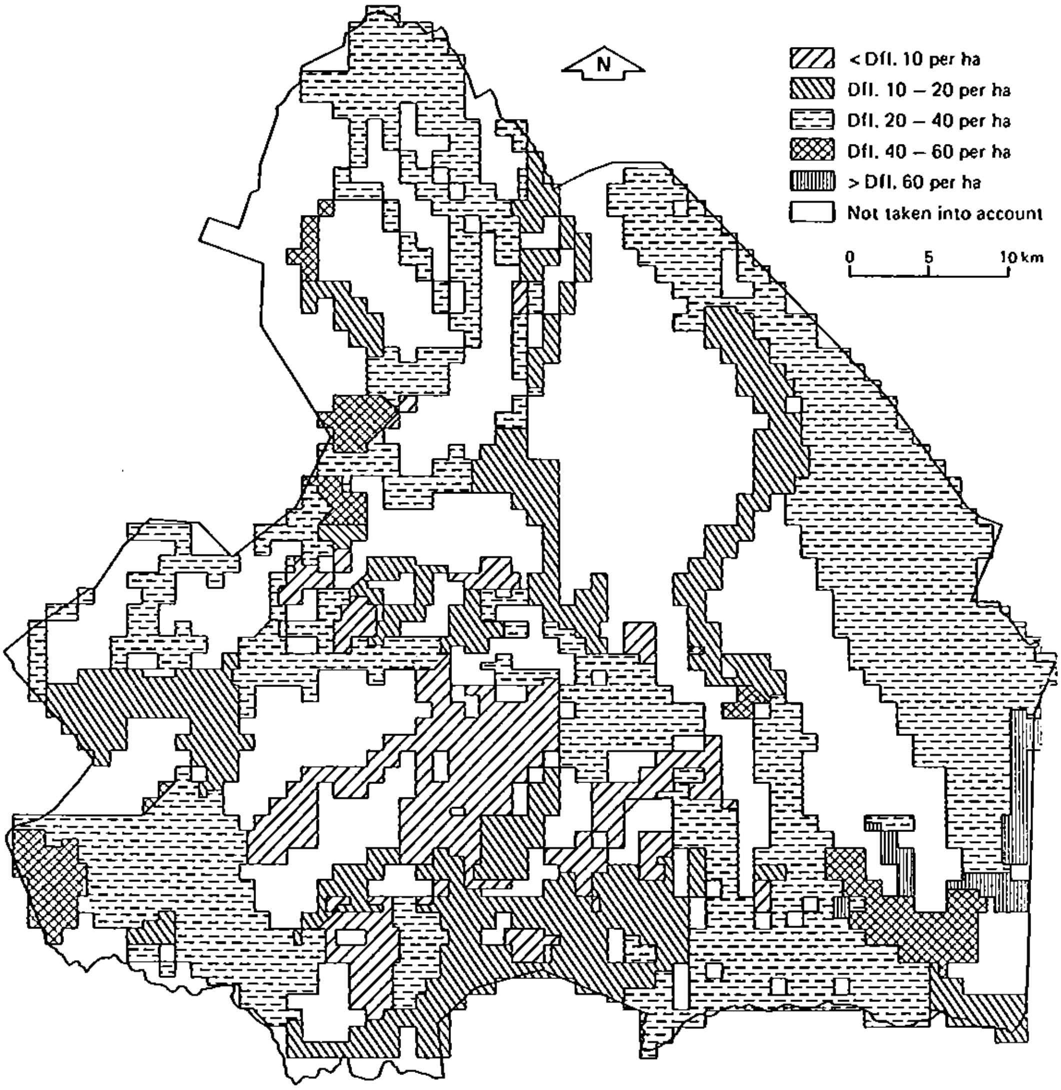

Fig. 12. Agricultural benefits ($Dfl.ha^{-1}$) of external water supply within the area of interest as evaluated by simulation (after WORKING GROUP 'TUS-10-PLAN', 1988).

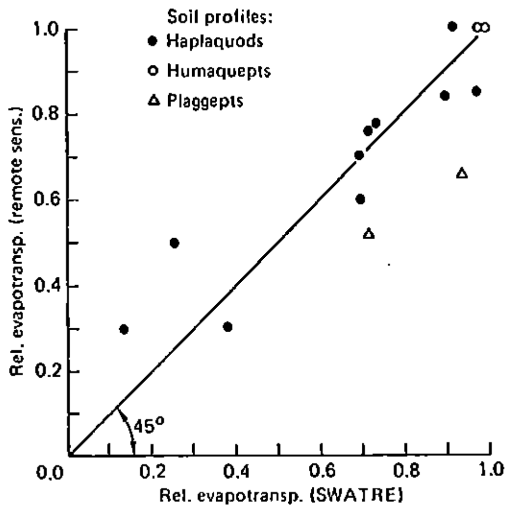

Fig. 13. Relative 24-hour evapotranspiration rates ET_a/ET_p as obtained by the remote sensing approach and calculated with the SWATRE-model for 14 grassland plots on three different soil profiles (after NIEUWENHUIS, 1986)